

# ENERGY INNOVATION











Brookhaven National Laboratory



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# **ENERGY INNOVATION**

## Brookhaven National Laboratory

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# ENERGY INNOVATION

# Brookhaven Lab tackles the nation's energy challenges

Global energy consumption is expected to surge more than 50 percent by 2035, as world population continues to increase and the technology that makes such development possible becomes increasingly widespread. But this energy comes at a significant cost. Our existing energy infrastructure cannot easily accommodate the expected increased demand and its accompanying environmental footprint. The most promising solution: Shift away from fossil fuels to sustainable, low carbon sources of energy and overhaul an electrical infrastructure — first designed and developed a century ago — to accommodate and integrate those sustainable sources.

The United States, which consumes about 20 percent of total global energy, is singularly equipped to lead the world in developing breakthrough innovations that could meet the challenges inherent in transitioning to a more sustainable energy portfolio — and doing so in ways that avoid deeper economic and environmental trade-offs. Investments in science — such as those from the U.S. Department of Energy (DOE) that fuel the fundamental research and unique facilities at Brookhaven National Laboratory — are the key. Basic and applied research conducted by Brookhaven scientists will lead to fundamental, game-changing solutions that address the region's — and the nation's current and future energy needs.

#### **Challenges and Opportunities**

In 2011, DOE embarked on an effort to establish a framework for transforming the nation's energy system. The result, called the Quadrennial Technology Review, identified two main energy challenges: The first involves transportation and energy security, as the U.S. currently sends \$1 billion out of the country each day for foreign oil, while the second involves the residential, commercial, and industrial sectors, and providing heat and power in environmentally responsible ways that strengthen U.S. competitiveness and protect the climate. In this context, the Review promotes a framework that focuses on six strategies:

- Increase vehicle efficiency
- Electrify the vehicle fleet
- Deploy alternative hydrocarbon fuels
- Increase building and industrial efficiency
- Modernize the grid
- Deploy clean electricity



New lenses made at Brookhaven Lab will focus light to within a single nanometer — one billionth of one meter — and open unprecedented possibilities for energy innovation.

Brookhaven Lab and its partners are working in many of these areas to transcend the limitations of current technology and solve grand challenges in energy. Long-term solutions will come from fundamental advances in basic science — new understanding of materials that generate, transmit, and store the energy we rely on more and more every day — and in translating those advances into marketable technologies.

Brookhaven's energy research portfolio focuses on clearing the technological hurdles standing in the way of a lowcarbon energy economy. Although there are many aspects of the carbon challenge, most scenarios point to two key pathways for success: replacing fossil fuels with low- or zero-carbon alternatives, which would lead to an increase in electricity usage and a need for a vastly more efficient electrical infrastructure; and sustainable chemical conversions, which would use renewable energy sources to convert abundant materials, such as carbon dioxide or water, into higher energy materials, like ethanol or hydrogen.

Brookhaven is leveraging its world-class scientific staff, one-of-a-kind facilities, and key partnerships in New York State and beyond to target two overarching areas of research on these pathways — science and technology for electrical infrastructure, and science and technology for sustainable chemical conversion. These developments will address challenges at all points in the energy pipeline, from energy generation to end use, with a particular focus on technologies for energy transmission and storage.

#### **Transmission**

The nation's aging electrical grid faces significant challenges in terms of capacity, reliability, quality, and efficiency. Brookhaven scientists are looking for ways to improve this system through a range of basic research initiatives. For instance, they are exploring new classes of superconductors, which transmit electricity without loss. Just one transmission cable made from these superconducting materials could take the place of 10 conventional copper transmission lines, and require 1,000 times less rare earth



Brookhaven scientists use advanced techniques including electronbeam lithography to synthesize catalysts, solar cells, and other new materials with nanoscale precision.

metal. Researchers are also probing superconductivity on the fundamental scale, working to decode the physics behind this hyper-efficient, loss-free phenomenon in the hope that such understanding will lead to more widespread energy-transmission applications.

#### **Distribution**

Through the Lab's participation in the Smart Grid Consortium and other partnerships, Brookhaven is helping to increase the efficiency and reliability of the electrical distribution system. By advancing measurement technologies and pioneering materials and systems for grid-scale storage, researchers will help lower electricity costs while ensuring that power is available when needed in the densely populated Northeast. These technologies will be key to managing peak energy demand, as well as swift recovery following outages caused by natural disasters and other unforeseen events.

#### Storage

Large-scale energy storage is essential to reliably harnessing variable sources

such as sunlight and wind and integrating them into the grid that distributes electrical energy to end users. To compensate for cloudy days and offshore lulls, Brookhaven is developing a new generation of superconducting magnetic storage systems that can hold massive amounts of electricity without the characteristic losses of existing technology. On a smaller scale, Brookhaven researchers are studying new materials that can leapfrog the limitations of today's portable batteries. Research at our Center for Functional Nanomaterials plays a large role here, as batteries (chemical storage) and capacitors (physical storage) based on nanostructured materials offer a new paradigm for portable energy. Brookhaven's own micro-grid and solar array will serve as a testing ground to perfect these new technologies.

#### Generation

Scientists estimate that 600 million megawatts of **solar power** — equivalent to the output of more than half-a-million typical coal-burning power plants — could theoretically be captured and used

on Earth. With experiments at our Center for Functional Nanomaterials, Brookhaven scientists aim to increase the efficiency and lower the cost of photovoltaic cells by developing new synthesis techniques and greater fundamental understanding. The Lab also hosts a dedicated photovoltaic research array, formed in partnership with the Long Island Solar Farm, to test utility-scale solar energy installations. The sun may also be used to directly produce alternative fuels through novel processes of artificial photosynthesis being developed by chemists at the Lab.

Wind power is expected to be the fastest growing electricity generator over the next two decades. Brookhaven scientists are pioneering new high-temperature superconductors to radically raise efficiency and diminish the need for costly rare earth metals in offshore turbine technology.

Brookhaven scientists are engineering catalysts that can distill and harness pure **hydrogen**, an abundant and clean-burning element that could revolutionize fuel industries. Scientists are also developing catalysts to optimize **biomass** conversion, which transforms renewable organic plant matter into combustible gas or liquid fuels. Brookhaven biologists are also exploring strategies for engineering plants optimally tailored for biofuel production.

**Nuclear** power, responsible for a quarter of the electricity in New York State, will play a key role in a future of lower emissions, but reactor safety is of paramount concern. Brookhaven is developing nanomaterials specially suited to function in high-radiation environments that will make nuclear energy safer than ever.

#### Use

Brookhaven Lab scientists have been re-engineering the costly and sensitive catalysts essential to the emerging fleet of electric vehicles. By probing materials with atomic-level precision using tools at our National Synchrotron Light Source and developing novel nanocatalyst structures at our Center for Functional Nanomaterials, Brookhaven researchers have radically diminished the amount of platinum typically needed and increased the efficiency and durability of environ-

mentally friendly fuel cells. These technologies, a clear example of basic research informing applied design, are already being mobilized by the Lab's partners in the auto industry.

#### **Technology Pipeline Strategy**

Brookhaven's new energy technologies are developed through a distinct "discovery to deployment" process. Marketable products are the end result, but they begin with an idea or discovery developed through basic research, the cornerstone of innovation

and our best opportunity to develop breakthrough solutions.

Brookhaven researchers work with industrial, academic, and commercial partners to identify a particular scientific problem that needs to be solved, then use the Lab's unique scientific facilities to explore the fundamental physics, chemistry, or biology involved and develop a technology solution. We then work with those industrial/commercial partners to move the new technology into the marketplace.



#### The Energy Challenge in New York and the Northeast

New York State, home to one of the world's largest cities, faces unique challenges, but it has also had singular successes in handling its population's energy demands.

It's the most energy-efficient state in the continental U.S. on a per-capita basis, with 6.3 percent of the nation's population accounting for only 4.3 percent of its total energy consumption. New York has been very aggressive in terms of carbon reduction, and derives only 4.4 percent of energy from coal as compared to 23.6 percent nationally. But New York still relies on fossil fuels, getting nearly a third of its electricity from natural gas.

In terms of challenges, most of New York State's energy is generated upstate and then transmitted some distance downstate to the main population centers, which creates congestion and an inefficient bottleneck for electricity distribution. Meanwhile, the city itself is too densely developed to easily accommodate the major public works programs needed to overhaul the aging electricity infrastructure beneath its streets. Variations in power quality and reliability can hurt manufacturing through down time and blackouts. And since large-scale energy storage has

yet to become a widespread reality, utilities must constantly run power plants at a high percentage of capacity to meet peak loads that only occur for about 100 hours a year, and struggle to easily integrate variable-output sources of renewable energy, like the wind and sun, into the mix.

The biggest challenge for NY State will be meeting the lofty goals it has set for itself. In 2009, the governor of New York signed an executive order requiring a reduction of all greenhouse gas emissions within the state to a level 80 percent below 1990 levels by 2050. With most of the "low-hanging fruit" already gone, the state can meet those targets only by powering more vehicles with electricity, increasing the capacity and reliability of the grid, and replacing fossil fuel-generated electricity with sustainable, low-carbon alternatives.

These needs align very closely with Brookhaven Lab's energy programs, and New York and the Northeast are a key focus of our efforts to overhaul the electrical infrastructure and develop new, sustainable sources of low-carbon energy — so the region represents an ideal testbed for the technologies developed at the Lab.



Stony Brook University's Advanced Energy Center

# PARTNERS IN DISCOVERY

### Working together to solve energy challenges

Brookhaven is working in partnership with an extensive network of collaborators and consortia in New York State to address electric infrastructure needs, challenges, and opportunities that are especially important in the Northeastern United States.

The success of Brookhaven Lab's energy research program is directly tied to the strong relationships we've developed with industry, academia, and government/not-for-profit agencies. These partners, and the shared resources they can bring to bear on scientific problems, are key to identifying and solving grand challenges in energy.

#### Stony Brook University

As one of the managing partners of Brookhaven National Laboratory and the source of its largest facility user base, Stony Brook University has strong ties to the Laboratory, especially in the area of energy research. The Laboratory and Stony Brook have made a series of joint staff appointments in computing, energy storage, condensed matter physics, materials science, and biology that are fostering increased collaboration and synergy. The two institutions are also partnering on large-scale grid-related and energy storage initiatives that have the potential to enable game-changing advances in these areas.

The first of these, the Smarter Grid Research Innovation, Development, Demonstration, Deployment Center (SGRID<sup>3</sup>) will serve as a "grid laboratory" and operate out of a new facility at Brookhaven

to be called the Advanced Electrical Grid Innovation and Support Center (AEGIS) and the NY State Smart Grid Innovation Center, to be built at Stony Brook. The second is a new battery hub, planned to operate out of Stony Brook's Advanced Energy Center, which will focus on developing new chemistries and extended lifetimes for batteries used in grid storage and electric vehicle applications.

#### New York State Energy Research and Development Authority

Brookhaven works closely with the New York State Energy Research and Development Authority (NYSERDA). This one-of-a-kind, very active public authority is seen as a model for public/private partnerships across the country. Funded by utility ratepayers, NYSERDA has been very successful in helping New York meet its energy goals by reducing energy consumption, promoting the use of renewable energy sources, and protecting the environment.

#### New York Battery and Energy Storage Technology Consortium (NY-BEST™)

The NY-BEST Consortium was created in 2009 to position New York State as a global leader in energy storage technology, including applications in transportation, grid storage, and power electronics. As the only national laboratory in the region, Brookhaven is poised to make important contributions.

## New York State Smart Grid Consortium and Utilities

The challenge of electricity delivery in the Northeast is one of meeting dense urban demand with widely distributed generation: How do we reliably supply electricity to very dense population centers with limited generation and an aging distribution infrastructure? To meet this challenge, Brookhaven has joined with other key stakeholders in the New York State Smart Grid Consortium (NYSSGC), founded in 2008 as a non-profit, public-private partnership to harness the state's unique resources to promote broad statewide implementation of the smart grid.

The Lab's connections with NYSSGC and NY-BEST provide a solid connection to the energy storage needs of real utilities — namely efficient transmission and especially distribution to enable effective management of peak energy demand, integration of renewable energy, and enhanced reliability.

Brookhaven is working closely with energy utilities, including the Long Island Power Authority (LIPA) and Orange and Rockland Utility (ORU), on strategies to enable more efficient and reliable transmission and distribution of electricity in our densely populated region. ORU is a leader in the use of new modeling technologies that allow for more accurate prediction of consumer demand and peak electrical load under a variety of conditions. LIPA's transmission system was among the first to demonstrate the feasibility of high-temperature superconductor wire technologies, and the utility is currently working with Brookhaven to enable integration of new energy sources into the grid.

#### **Broader University Community**

Brookhaven has established dynamic collaborations with universities across NY State and the Northeast that share a common interest in solving particular energy problems and challenges. Through their participation or leadership in four DOE Energy Frontier Research Centers, Brookhaven scientists are working with researchers at Rensselaer Polytechnic Institute, Columbia University, Cornell University, the State University of New York at Binghamton and Buffalo, and other regional educational pillars to make breakthroughs in superconductivity, photovoltaics, energy storage, and other areas.

#### Industry

The energy challenges we face will require, at a minimum, new approaches to energy systems, and in most cases will require the development and deployment of new technology. Brookhaven is working closely with industrial giants like General Electric, General Motors, and others to both determine the specific needs of those using a particular technology, and to foster a better understanding by industry of the unique facilities and skill sets available at the Laboratory. The overall goal is to build deliberate "discovery to deployment" pipelines that incorporate feedback and input from industry at each step of the development process.

Brookhaven is taking advantage of all the technology transfer opportunities available to expand its impact on the marketplace, including the new Agreement to Commercialize Technology mechanism, which is expected to make it easier for companies and other research organizations to enter into collaborations with the Laboratory.





# CARBON-FREE GENERATION AND INTEGRATION

Improving materials to make the most of wind, solar, and nuclear power

Scientists at Brookhaven are leading efforts to develop a range of new materials to overhaul wind turbine generator construction and design, improve the efficiency of solar cells, and outlast the harsh conditions in nuclear reactors.

From the earliest fires of civilized man to the coal furnaces of the industrial revolution, carbon has been an essential source of energy and driver of progress. But carbon-based fuel produces energy only at the cost of significant pollution. The carbon dioxide gas released by burning fossil fuels, including natural gas and refined petroleum, plays a leading role in greenhouse gas emissions and the rising threat of ocean acidification.

For decades, forward-thinking industries and innovators have been marching toward a carbon-free energy future, an era fueled by sustainable resources. Decarbonized generation will be the backbone of 21st Century energy innovation.

#### Polymer/Thin Film Solar Cells

The accelerated development and large-scale integration of solar energy solutions may hinge on polymer-based semiconductor solar cells. These lowcost and highly scalable organic materials offer significant advantages over their inorganic counterparts, including strong optical absorption and synthesis on flexible substrates. These devices are typically made by blending together a polymer electron donor with an electron acceptor material to create a nanostructured composite with high interface density. Researchers apply the polymer blend as a thin film sheet between two conducting metal electrodes. Sunlight generates electronic excitations within the organic semiconductor in the form of electron-hole pairs, and these custom-grown films enhance the subsequent flow of electrons and holes to generate electricity.

Scientists at Brookhaven have been leading efforts to understand the relationship between the molecular structure of polymer semiconductor

materials and their ability to efficiently convert sunlight to electricity. In one series of experiments, scientists structured the material with an embossing technique called nanoimprinting, which stamps organic polymers with patterned grooves measuring just 50 nanometers. The nanoscale synthesis, carried out at Brookhaven's Center for Functional Nanomaterials (CFN), imparts a sense of molecular order in the polymer chains, creating oriented configurations that can improve solar-cell performance. In other experiments, researchers demonstrated that confining the blended solar material within nanoscale pores allowed for 500 times greater electrical conductivity, resulting in solar cells with twice the electricity output for the same amount of absorbed sunlight.

X-ray diffraction measurements at the National Synchrotron Light Source (NSLS), which map nanoscale structures based on the way high-intensity x-rays bounce off materials, played a crucial role in understanding and improving polymer performance in these studies. Brookhaven Lab scientists conducted additional detailed structural studies of some of the best-performing photovoltaic polymer semiconductors, including the highly active material PCDTBT. X-ray diffraction revealed an unexpected bilayer microstructure that may help explain that promising polymer's superior performance at converting sunlight into electricity.

#### Solar Array Studies

Brookhaven Lab is committed to exploring technological advances that will both generate more renewable energy and allow it to be effectively integrated into the existing electric grid. The geographically dispersed and unpredictable character of many renewable energy sources such as wind



Brookhaven uses synchrotron characterization techniques for the in-situ study of materials for advanced energy systems.



and solar presents major challenges for seamless, efficient management of electricity transmission and distribution. Two facilities on the Brookhaven site will help advance that research.

Brookhaven Lab hosts the Long Island Solar Farm (LISF), a 32-megawatt solar photovoltaic power plant built through collaboration between BP Solar, the Long Island Power Authority (LIPA), and the Department of Energy. The LISF began delivering power to the LIPA grid in November 2011 and is currently the largest solar photovoltaic power plant in the Eastern United States. With such close proximity to the LISF, Lab researchers are studying the challenges of deploying large-scale solar power installations in the Northeast, where variable weather can impact

the array's output. Predicting solar array performance will help integrate and manage power from other renewable but similarly intermittent sources.

As the solar panels at the LISF collect energy, researchers at Brookhaven monitor sensors and analyze large amounts of data from the LISF systems. The data will be used by researchers at the Lab and across the country to address the key issues facing deployment of large-scale solar power plants.

A separate seven-acre research array, central to the new Northeast Solar Energy Research Center (NSERC), will allow engineers and scientists to study innovative new technologies and increase the economic competitiveness

of utility-scale solar plants. Construction of the 1-megawatt, reconfigurable research array should be completed in the summer of 2013. This DOE-owned facility will be a proving ground for Brookhaven Lab and its industrial partners to test new solar technologies, including electrical inverters, storage devices, and solar modules.

### Superconducting Wires for Wind

Today, all electricity generators require coils of wire, often copper, to conduct electric current. Massive wind farms with multi-ton turbines are no different. In direct-drive turbine generators, high-energy-density permanent magnets create high magnetic flux densities to efficiently convert torque into electricity. But popular turbine technologies use rare-earth materials such as neodymium and dysprosium, which are in short supply and mostly imported. While mineral deposits in the U.S. contain many rare-earth elements, China provides over 95 percent of the worldwide supply of these materials. With increased global competition, reliance upon a single, limited source presents a "critical risk" to domestic technology development.

In a project funded by \$1.4 million from ARPA-E (Advanced Research Projects Agency-Energy), Brookhaven Lab and AMSC (formerly American Superconductor Corporation) are developing new technologies to overhaul wind turbine generator construction and design. AMSC, responsible for nearly 10 percent of the world's wind-generated electricity, lends industrial and commercial expertise to the scientists and cutting-edge research facilities at Brookhaven. The trick to achieving an ideal performance-to-cost ratio in wind energy is developing high temperature superconducting (HTS) wires.



The Long Island Solar Farm, located on the Lab site, offers research and field-testing capabilities under actual northeastern weather conditions — leading to crucial advances in solar forecasting and grid integration.

With near-zero electrical resistance, HTS wires wound into rotor poles produce high torque very efficiently and deliver twice the power of a conventional turbine at just one-half the size. HTS wires eliminate nearly all rare-earth content, and the increased magnetic flux density of the coils enables lighter, less-expensive structures and more simplified assembly. For HTS-based technology to become the preferred choice for offshore wind turbines, large wires must be synthesized that set a new standard for current density and industrial-scale construction. Brookhaven's Advanced Energy Materials group is designing catalysts and new synthesis processes for custom, cost-effective, high-performing superconductors. Using the materials analysis possible at the NSLS and electron probes at the CFN, Brookhaven researchers are clearing the way for wind.

#### Nuclear Energy Systems/ Advanced Materials for Radiation Environments

As the economy shifts away from its fossil fuel dependence, the maintenance and possible expansion of nuclear power will play a key role. The same fission activity that creates energy in nuclear reactors also causes damage to its components, affecting efficiency, cost-effectiveness, safety, and longevity. The next generation of reactors will operate with even higher temperatures and higher fluxes, leading to the accelerated degradation and eventual failure of key core materials through corrosion, cracking, and swelling.

Brookhaven Lab is uniquely positioned to address these pressing challenges and enhance the safety and sustainability of nuclear energy. Researchers use the Brookhaven Linac Isotope Producer (BLIP) to simulate the effects of radiation

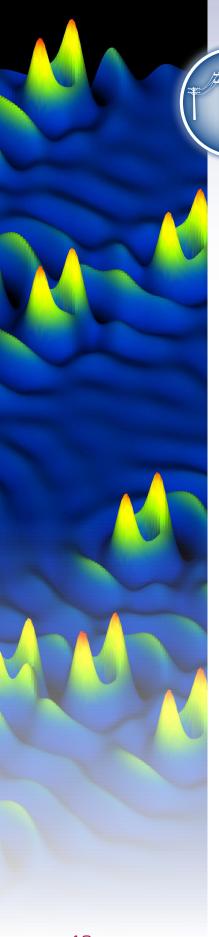
#### **Distributed Energy Generation**

Brookhaven scientists are especially interested in the challenge of distributed generation — power from multiple sources distributed across a region — and how it will impact the efficiency and reliability of electricity delivery. For the past century, large centralized power sources generated most electricity, which was then delivered to customers through the distribution grid of transformers, power lines, etc. With distributed solar energy sources as large as the LISF and as small as arrays installed on roofs of homes being connected to the grid, electricity from multiple sources with the possibility of two-directional power flows must be smoothly integrated. This multi-directional power flow can create control and stability issues within the existing grid. Another rising question is the effect on the electric grid of solar energy fluctuations, caused by clouds and the sun's influence as it rises and sets. Research at Brookhaven will help address these and other emerging issues related to the grid integration of renewable energy resources.

on the materials. Scientists then use instruments at NSLS and CFN to probe nanostructures and reveal atomic behavior underlying material behavior in a range of extreme environments.

Through a series of irradiation and high temperature experiments, researchers confirmed that applying nanostructured coatings of specific materials — amorphous iron, aluminum, titanium, and combinations thereof — enhances the ability to resist radiation damage, sustaining flexibility for longer periods than materials without custom nano-coats. The mechanism behind this phenomenon is not fully understood, but active investigations are unraveling the mystery.

Other customized nanomaterials have high interface content, allowing them to absorb high levels of radiation damage and leave a "healed" material. Researchers at CFN explore these selfhealing materials, including copper niobium, subjecting them to high temperatures and bombarding them with helium and krypton radiation. Additionally, promising nanoporous metal-organic materials are being tested for their ability to absorb fission gases without substantial degradation. This intense experimentation on a range of nuclear core materials will improve the safety and efficiency of current and future power plants.



# ELECTRIC POWER TRANSMISSION AND DISTRIBUTION

Designing new methods to deliver power to homes and businesses

Working with a range of collaborators from key industry, government, and academic institutions, Brookhaven Lab is developing a set of facilities, programs, and fundamental technology innovations to advance the next-generation electric grid. This research is building a signature bridge between basic science and technology deployment.

As sustainable energy generation advances and new alternative fuel sources emerge, aging electrical infrastructure must evolve as well. Renewable energy innovations must be supported by new methods to deliver that power to homes and businesses. Brookhaven Lab and its partners are investing heavily in efforts to push the fundamental technology underlying electricity transfer into an era of unprecedented efficiency and sustainability. These advances are especially crucial to New York State, where dense urban populations and climbing energy demands challenge large-scale renovations.

#### Second-Generation HTS Wires

Loss-free, low temperature superconductors suffer from an unfortunate stumbling block: They only function at temperatures near that of liquid helium, very close to absolute zero. The energy used to cool superconducting wires often offsets what might be saved in transmission. But hightemperature superconductors (HTS) perform at the relative warmth of liquid nitrogen and carry high amounts of current with a much smaller footprint, making them more viable for widespread grid applications. With helium reserves in short supply, the ability to use nitrogen, by far the most abundant gas in our atmosphere, would be another major benefit.

Brookhaven Lab and its industrial partners lead the way in making HTS wires economically viable, actively linking basic research with commercial deployment. The Advanced Energy Materials Group is working to increase the electric current density of secondgeneration (2G) HTS wires by 400 percent, and an ongoing collaboration with American Superconductor Corporation has already achieved a 50 percent increase. In addition, they hope to reduce the need for rare-earth metals by a factor of 1000, moving past the traditional large-scale permanent magnets that can generate a comparable magnetic field.

The trick to achieving this dramatic technological improvement, which would immediately impact technology ranging from wind turbines to grids, is a nanoscale technique called the synergistic flux pinning approach. The subtle motion of magnetic flux lines in most HTS materials causes electrical

resistance and instability. To prevent this, Brookhaven Lab scientists grow these remarkable materials with a proprietary process that not only engenders native flux pinning nanostructures, but also precisely controls the synthesis process and quickly finetunes each element. This technique, currently applied to the promising HTS compound yttrium barium copper oxide, is singularly scalable for low-cost industrial production of the long-length wires essential to overhauling our energy transmission infrastructure.

Brookhaven's outstanding edge in advancing high-current-density 2G HTS wires is the close proximity of multiple cutting-edge facilities on site. The ultraviolet photon spectroscopy available at the National Synchrotron Light Source (NSLS), transmission electron microscopy at the Center for Functional Nanomaterials (CFN), and area-specific low energy electron diffraction (LEED) and microscopy (LEEM) instruments all combine to provide an unparalleled capability to identify structures and morph-

ologies, and determine the exact initial growing conditions of the HTS wires. Brookhaven pioneers some of these proof-of-principle HTS production techniques, which industrial partners can then scale up and move into grid-scale environments.

Beyond that applied work of materials synthesis, scientists at Brookhaven's Center for Emergent Superconductivity also explore the most fundamental quantum-scale physics underlying high-temperature superconductivity. Using a custom-built molecular beam epitaxy device, researchers are building atom-thin materials and probing the propagation of magnetic waves that could explain the electron coupling behind loss-free transmission. Exploring this uncharted fundamental territory may unlock the recipe for superior superconductors that function even at room temperature.

#### **Building a Smarter Grid**

The nation's electrical transmission and distribution system currently experiences losses that range from eight to 11 percent,

#### Partnering with Utilities on the Smarter Grid

One goal of the "smarter" grid tools under development at Brookhaven is to reduce electricity distribution losses by as much as 50 percent. Brookhaven has hosted representatives from several Northeast utilities for a demonstration of a new modeling technology — already being used in several locations - that may help accomplish this goal. Virginia Tech's Integrated System Model/Distributed Engineering Workstation (ISM/DEW) will allow the grid to move from a static mode, where planning is based on a single data point, to a total of 8,760 data points every hour, 24 hours a day, for a full year. This new model can quickly compile power-use and generation data, taking into account all the different components on the utility's grid. Central Hudson Gas & Electric (CHGE), an early adopter of the smarter grid concept,

is also using an approach similar to that of Orange and Rockland Utility (ORU) to make its power system more robust, cost effective, and better able to accommodate renewable generation. Its use of ISM/DEW in concert with control of solar integration technologies will allow CHGE to maximize its penetration of customer-owned solar in its service area.

Brookhaven is also working with the Long Island Power Authority (LIPA) to use probabilistic risk assessment methodologies to assist in decision-making and management of assets and investments. This is particularly helpful in emergency response situations where immediate cost/benefit decisions are needed regarding replacement/repair of equipment.

# Energy Frontier Research Center – Center for Emergent Superconductivity

Brookhaven Lab hosts one of the Department of Energy's Energy Frontier Research Centers (EFRCs), which are dedicated to laying the scientific groundwork for fundamental advances in solar energy, biofuels, transportation, energy efficiency, electricity storage and transmission, clean coal and carbon capture and sequestration, and nuclear energy. EFRC researchers are exploring cutting-edge capabilities in nanotechnology, high-intensity light sources, neutron scattering sources, supercomputing, and other advanced instrumentation. Brookhaven's EFRC, with annual funding of \$2.5 million and led alongside partners at the University of Illinois and Argonne National Lab, takes full advantage of the unique research strengths of the National Synchrotron Light Source (NSLS) and the Center for Functional Nanomaterials (CFN), which probe materials at scales approaching one billionth of a meter.

The Brookhaven EFRC, dubbed the Center for Emergent Superconductivity, seeks to understand the fundamental nature of superconductivity in complex materials. Unlike ordinary conductors, superconductors carry current with zero resistance, so that no electricity is lost as it travels along wires from power plants. Collaborating scientists are exploring methods to improve the critical properties of known superconducting materials and accelerate the search for new ones. This EFRC research is ultimately aimed at improving the capacity, efficiency, and reliability of the electric grid. Energy delivery is a crucial issue for New York and the nation, especially as substantial renewable energy sources like the sun and wind are integrated into the existing system.

with most of those losses occurring in the distribution system that delivers electricity to homes, commercial businesses, and industry. Brookhaven Lab is focused on developing tools to move us toward a "smarter"grid — one that will be able to automatically respond to changes in generation and load profiles and provide more efficient electricity delivery. Our goals are to reduce the cost of electricity in New York State and the Northeast by advancing sensing and measurement technologies,

developing simulation tools for robust grid management, enabling increased distributed generation using advanced materials, and supporting expanded use of energy storage.

The challenge of improved electricity delivery in the Northeast is one of meeting dense urban demand with widely distributed generation: How do we reliably supply electricity to very dense population centers with limited generation and an aging distribution

infrastructure? To meet this challenge, Brookhaven has joined with other key stakeholders in the New York State Smart Grid Consortium, founded in 2008 as a non-profit, public-private partnership to harness the state's unique resources to promote broad statewide implementation of the smart grid. It is the only organization of its scale in the nation committed to representing all major contributors across the energy value chain from utilities, markets, operators, industry, academia, government and end-users. Working with the Consortium and other key industry, government, and academic institutions, the Laboratory is developing a set of facilities, programs, and tools to advance the next-generation electric grid.

#### SGRID<sup>3</sup>: New York's Smart Grid Laboratory

With the support of a \$5 million grant from New York State, Brookhaven Lab and Stony Brook University have collaborated to form a "grid laboratory" — the Smarter Grid Research, Innovation, Development, Demonstration, Deployment Center (SGRID<sup>3</sup>).

SGRID<sup>3</sup> will operate out of the Advanced Electric Grid Innovation and Support Center (AEGIS), a new facility proposed for construction at Brookhaven, and the Advanced Energy Research and Technology Center at Stony Brook. Both will be augmented by construction of a NY State Smart Grid Innovation Center at Stony Brook. These facilities and their focused research and development work on smart grid technologies will be supported by the two institutions' leading-edge science and technology facilities and world-class staff, and will leverage their relationships with a unique array of energy-related organizations and assets in New York State.

SGRID<sup>3</sup>'s primary goals include:

- Lowering the cost of electric power by five to 10 percent and improving the quality and reliability of electric power on Long Island and in NY State
- Accelerating breakthrough technologies in smart grid devices and the future construction, operation, and control of electric power transmission and distribution systems
- Creating an infrastructure for developing and testing new grid technologies, equipment, and components that will contribute to economic growth through creation of spin-off companies that will, in turn, create new, highincome jobs on Long Island and throughout New York State
- Developing knowledge that will guide future utility investments in the electrical transmission and distribution systems in New York State, with a strong focus on improving storm preparation, response, and recovery related to hurricanes and other extreme weather events

Important components of the AEGIS project include a collaborative effort with the Long Island Power Authority (LIPA) studying the reliability of LIPA's east-end distribution feeder, and work with two upstate utilities to use their models and feed their real-time electric grid information into AEGIS.

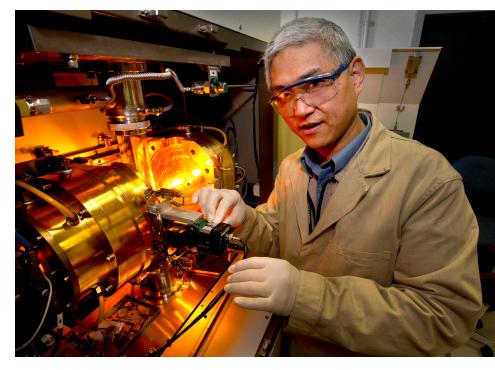
## Microgrid Demonstration Project

NSERC, the Lab's on-site solar research array, will enable the use of a portion of the Lab's campus as a test bed for smart grid technologies, such as smart grid sensors. One of the Lab's key tools for advancing the smart grid, this on-site "microgrid" can be used by researchers, utilities and industry as a test bed for new transmission, storage, sensing, and integration technologies. A microgrid is a self-contained electricity production and distribution system that includes distributed generation (solar, wind, fuel cells), distributed loads (buildings, data centers, street lights), and electricity storage, maintained in balance through advanced sensing and controls while in isolation from the larger grid.

With the assistance of Virginia Tech and the Canadian company Smart Energy Instruments, the Lab will examine the applicability of "smarter" grid sensors to better monitor and manage distribution networks like ours. The project will use the Laboratory's large electricity

distribution infrastructure as a utilityscale microgrid, a "laboratory" for testing and demonstration, facilitating more widespread use of distributed generation sources, such as solar and wind. Sensors deployed around the site will be used to try to gauge some of the power quality issues on site.

By observing how the Lab's grid works, researchers will be able to get performance data, analyze it, and bring together advanced modeling capabilities to learn how to use synergies to save power and improve efficiency. The NSERC solar test array will play a large role, as it will enable real-world, utility-scale tests of advanced "smart grid" ready technologies, such as electrical energy storage systems and smart grid-ready solar inverters, which should increase the ability of utilities to integrate solar energy into the grid.



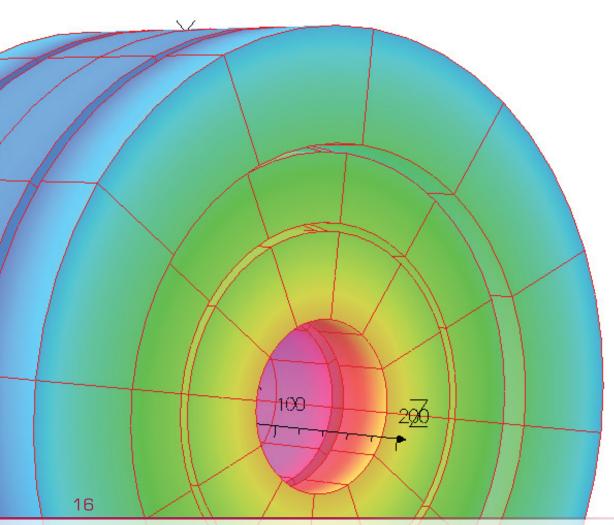
Brookhaven physicists grow single-crystal superconductors that could revolutionize the efficiency of electricity generation and transmission.



# ELECTRICAL ENERGY STORAGE

Building better batteries and new grid-scale storage systems

Improved energy storage could transform the electric grid to enable reliable integration of renewable energy sources and pave the way for more advanced electric vehicles.



**ENERGY INNOVATION at Brookhaven National Laboratory** 

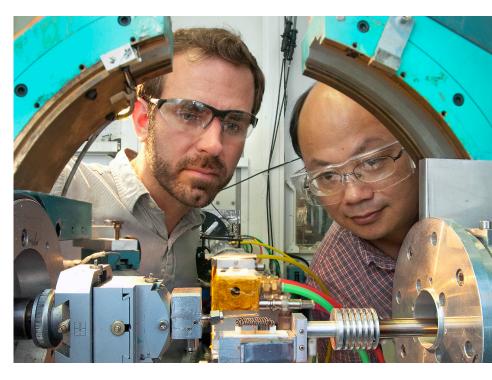
To significantly reduce our nation's reliance on fossil fuels for electricity generation and transportation, we must develop innovative electrical energy storage technologies. Improved energy storage could transform the electric grid to enable reliable integration of energy from intermittent renewable resources — like the sun and wind — and pave the way for more advanced electric vehicles with extended range for daily use.

To achieve these goals, Brookhaven is conducting basic and applied research with a range of industrial and academic partners. Their aim: develop more efficient, economical, and safe energy-storage materials and systems, with a focus on longer lifetimes, high energy densities, and fast cycling rates.

The limitations imposed by the lifetimes of existing energy storage materials and systems are a universal underlying barrier, with a major impact on cost, safety, and performance. To break through the lifetime barrier, we must close the critical gaps in our understanding of these materials and their functional interfaces at the nanoscale — the scale at which the fundamental chemical and physical interactions of energy transformations take place.

## Advancing Lithium Technology for Autos and Beyond

Increasing the use of hybrid electric vehicles, electric vehicles, and hydrogen fuel-cell vehicles is essential for reducing oil dependency. Brookhaven conducts leading-edge research into lithium batteries — the most widespread commercially available technology, particularly for transportation applications — to improve the affordability and safety of these vehicles, with a special focus on increasing battery lifetimes.



Brookhaven Lab researchers and their collaborators have developed methods of examining lithium-ion reactions in real-time with nanoscale precision.

Many otherwise promising high-capacity electrode materials are limited by lifetime issues. Material degradation during system use is at the root of battery-related cost and safety concerns. In the past decade, Brookhaven scientists have developed new electrolytes and electrolyte additives, and pioneered new x-ray absorption and diffraction technologies for battery material studies using the Lab's unique facilities, including the National Synchrotron Light Source (NSLS) and the Center for Functional Nanomaterials (CFN).

Brookhaven scientists are now developing new nanoscale electrode materials capable of higher lithium capacities and rapid cycling rates, both key for increasing performance. Alternative high-capacity anodes have the potential to double or triple cell capacity, but these materials are plagued by large

volume changes, which affect their durability, and phase transitions that limit cycle life. Brookhaven's studies show that electrodes prepared from nanocrystalline powders and nanofilms may be able to sustain large volume changes without particle breakup. These electrodes exhibit improved cycling capacity characteristics as a result of their nanoscale dimensions. In addition, the nanoscale particle dimensions also promote fast cycling rates, which means higher power capabilities and less time needed to recharge the battery. The new nanosynthesis and characterization facilities at the CFN give Brookhaven a unique opportunity to explore these atomicand molecular-level processes.

Brookhaven researchers are also looking to improve battery cathodes by developing materials that can "host" more lithium. In a typical cathode, the negative charge from the lithium is donated to a metal ion in a process called reduction. Normally, there is one metal atom for every lithium atom that is cycled in the battery. Since the metal atoms are heavy, this ultimately limits the capacity of the host material. The Brookhaven team is developing new cathode materials with metal ions that can accommodate two or more electrons — which would significantly increase electrode capacity and ultimately reduce the battery's size and weight.

Brookhaven scientists have also devised a new way of making defect-free cathode materials using an in-situ reactor made out of glass. This glass reactor allows researchers to probe the precursors of the reaction with synchrotron x-rays generated at the NSLS and monitor changes as the reaction takes place. Because they use a heating process that doesn't involve a lot of costly solvents, this method significantly reduces overall processing costs.

## **Exploring Alternative Battery Chemistries and Architectures**

While lithium ion-based batteries are currently in widespread use, scientists know that no single material or device is likely to provide a comprehensive solution to meet our future storage needs for both automobiles and the

grid. So Brookhaven has launched a program to develop and test alternative battery chemistries and storage architectures, including so-called "flow" batteries, which are particularly attractive to utilities for storing very large amounts of energy on the grid.

In a flow battery, liquid electrolytes mixed with energy-storing materials flow from a tank through an electrochemical cell that reversibly converts chemical energy directly to electricity. Scientists at Brookhaven are collaborating with researchers at the City College of New York and Massachusetts Institute of Technology (MIT) to investigate the materials and electro-

#### Collaboration with General Electric

Brookhaven's unique scientific facilities are playing a major role in our growing industrial partnerships in the storage arena. For example, research conducted at the National Synchrotron Light Source (NSLS) enabled General Electric (GE) researchers to understand in detail the internal chemical



GE Durathon batteries produced at the company's new plant in Schenectady, NY, for use in grid- and utility-storage applications. (Photo: GE)

reactions and associated structural changes of an actual commercial battery during realtime charging and discharging. GE made use of high-energy x-rays and a detector developed by Rutgers University to penetrate the battery and gain information about the chemical content of its interior. This research helped GE engineers fine-tune battery design and improve performance. As a result, GE moved the battery, dubbed "Durathon," into commercial production for transportation and grid-storage applications, and constructed a new mass-production factory in Schenectady, NY.

Recently, the New York State Energy Research and Development Authority (NYSERDA) awarded \$5.5 million for a three-year project led by GE Global Research to accelerate the development of sodium metal halide batteries. The team consists of researchers from four New York universities and Brookhaven. The characterization technique used to develop the Durathon battery will be used to enhance the next generation of these batteries through improved reliability, cycle life, and performance.

chemical processes that underlie the current performance and reliability limitations of flow batteries. In-situ characterization of these batteries, including synchrotron-based diffraction, microscopy, and scattering experiments, will help reveal the evolution of battery materials during use.

#### Superconducting Magnet Energy Storage Systems and the Grid

Developing affordable, large-scale energy storage systems would be a game-changing advance for the U.S. electrical grid. In particular, energy storage will be crucial in enabling the widespread use of two key renewable yet intermittent energy sources: wind and solar power. Several Brookhaven projects funded through DOE's Advanced Research Projects Agency-Energy (ARPA-E) are aimed at developing technologies that could offer electrical energy storage on the grid scale.

In one example, Brookhaven and three collaborating institutions are developing an advanced superconducting magnet energy storage (SMES) system that uses magnetic fields in superconducting coils to store energy with near-zero energy loss, instantaneous dynamic response, and nearly infinite cycle life. Cost-effective, grid-scale SMES systems would offer megawatt-hours of stored energy with an almost endless cycling capability. This represents a paramount advantage over alternative energy storage devices, which are severely limited in terms of lifetime and environmental constraints.

Conventional SMES systems are typically used as small-scale, short-term power devices designed to compensate for fluctuations in electrical power systems. The collaboration has proposed an ultra-high-field



Grid-scale energy storage innovations are key to ensuring reliable operation of the 21st Century electric grid and for the integration of renewable energy sources.

SMES-based storage solution that would bring down large-scale storage costs to a point where they would be comparable in cost per kilowatt-hour to conventional storage solutions. However, significant technology challenges must be overcome to develop such a system.

For one, the performance of each individual subsystem of the proposed SMES system must be propelled far beyond the present state-of-the-art. With more than four decades of experience in developing superconducting materials and building high-field magnets, scientists at Brookhaven are leading the design and development of the SMES magnet coil and superconducting switches.

#### **NY-BEST Partnership**

The Lab's connections with the New York Battery and Energy Storage Technology (NY-BEST™) Consortium

and the New York State Smart Grid Consortium provide a solid connection to the energy storage needs of real utilities — namely efficient transmission and especially distribution to enable effective management of peak energy demand, integration of renewable energy, and enhanced reliability. The NY-BEST Consortium was created in 2009 to position New York State as a global leader in energy storage technology, including applications in transportation, grid storage, and power electronics.

By bringing together New York's energy storage companies, universities, and government partners such as Brookhaven, NY-BEST will help build and promote a vibrant, world-class, advanced battery and energy storage sector in New York. As the only national laboratory in the region, Brookhaven is poised to make important contributions.





# NEW CATALYSTS FOR FUEL CELLS AND HYDROGEN GENERATION

# Engineering nanostructured compounds to power a fuel revolution

Brookhaven's electrochemistry group is developing new highly active, stable, and durable catalysts that can play a major role in reducing the cost and increasing the longevity of fuel cells for electric vehicles, while other catalysis research may usher in a future powered by clean-burning hydrogen fuel. Fuel cells have long been recognized as a promising source of clean energy, as they can power electric vehicles with high efficiency and little or no emissions. Inside a fuel cell, catalysts convert the intrinsic chemical energy of an abundant fuel source such as hydrogen directly into usable electrical energy. The byproduct from these catalyst-driven chemical reactions is water, not carbon dioxide or other pollutants that can threaten the environment. This "green" potential challenges researchers to develop optimal new compounds to power a fuel cell revolution. Brookhaven scientists combine expertise, worldclass facilities, theoretical analysis, and industrial partnerships to drive catalyst research forward.

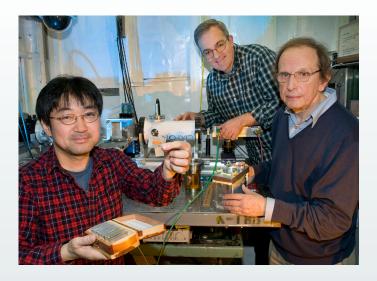
Platinum Monolayer Shell-Core Electrocatalysts

Brookhaven's electrochemistry group is developing new highly active, stable, and durable fuel cell catalysts that can play a major role in sustainable energy solutions. Before large fleets of fuelcell-powered vehicles can hit the road, scientists must find a way to protect top-performing platinum — the most expensive, fragile, and often-essential component of fuel-cell technology and to reduce the amount needed to make catalytically active electrodes. Beyond the price, platinum catalysts typically suffer from rapid deterioration during the stop-and-go driving common throughout the country.

Brookhaven's breakthrough platinum monolayer catalyst substantially reduces the technical obstacles in the way of durable, economical fuel cells. The custom-engineered nanoparticle opens the possibility to accelerate the commercialization of zero-emission hydrogen fuel cells for vehicles, as

well as other portable and stationary applications. The new catalyst reduces the rare and costly platinum required to a one-atom thick coating over less-expensive metals such as palladium and its alloys or other refractory metal alloys. On the atomic scale, the individual platinum atoms "feel"

the influence of the palladium atoms below, instead of platinum atoms. In a surprising discovery, experiments showed that not only was this novel core-shell structure stable, but the new palladium nanoparticles with platinum coats actually outperformed their expensive precursors.



# Partnering with Industry: N.E. Chemcat Licensing

The Department of Energy and its national labs actively collaborate with industrial partners to provide access to the breakthrough technologies developed by fundamental research. Brookhaven Lab's Office of Technology Commercialization and Partnerships coordinated one such key commercial licensing agreement to move these crucial nanocatalysts into practical application.

N.E. Chemcat Corporation, Japan's leading catalyst and precious metal compound manufacturer, has licensed Brookhaven's platinum-shell electrocatalysts to reduce the use of costly platinum and increase the effectiveness of fuel cells for use in electric vehicles. Beyond the nanoparticle design, the license also includes rights to innovative methods and custom apparatuses for catalyst synthesis. This model partnership facilitates the development of affordable and reliable fuel cell electric vehicles, which will benefit both the environment and consumers by reducing reliance upon nonrenewable fossil fuels.

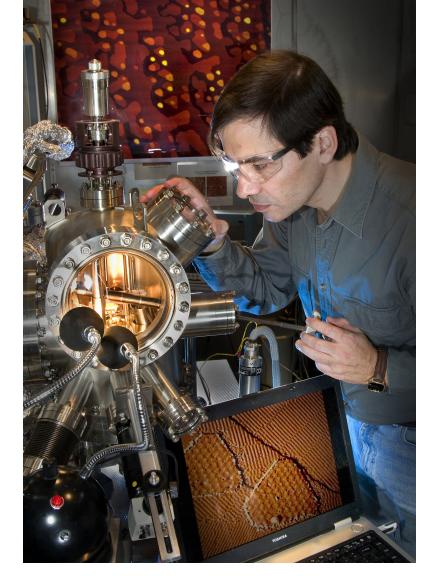
In another breakthrough innovation, Brookhaven researchers created low-cost, hollow, platinum-shell nano-catalysts without the typical metallic center. Scientists coated easily synthesized and abundant nickel nanoparticles with uniform layers of platinum about 2-3 nanometers thick. The nickel core was then dissolved, leaving a hollow sphere that actually compressed slightly around the empty space. The resultant low-platinum nanoparticle exhibited high durability and superior activity when compared to solid electrocatalysts.

Brookhaven scientists advance their fuel cell electrocatalysis concepts through strong cross-laboratory collaboration, combining the reaction analysis expertise of the chemistry group, high-intensity x-ray imaging at the National Synchrotron Light Source (NSLS), and electron microscopy and materials synthesis at the Center for Functional Nanomaterials (CFN).

## Purification Processes for Hydrogen Generation

Hydrogen, the world's lightest and most abundant element, may also hold the key to a sustainable energy future, from fueling chemical synthesis to powering automobiles. But tapping the potential of hydrogen requires absolute purity, and producing the element in isolation presents an ongoing challenge.

During a water-gas shift reaction, carbon monoxide and water vapor react to form carbon dioxide and pure hydrogen molecules — but an appropriate catalyst must facilitate the process. Brookhaven Lab researchers combined techniques including photoemission, time-resolved x-ray diffraction, and



Scanning tunneling microscopes reveal the structural details of new catalysts, providing key clues for the development of breakthrough technologies.

x-ray spectroscopy at NSLS to identify the structure and reactivity of high-performing catalytic compounds of materials such as titania, ceria, and gold or platinum nanoparticles. Further experimentation revealed an even better performing catalyst, as measured by its production of hydrogen, which substituted less-expensive copper for gold. The reaction mechanics are still under investigation, and each successive round of synthesis, experimentation, and nanostructure analysis advances the technology.

Carbon monoxide is itself a harmful emission, and harnessing it to chemically produce hydrogen actually increases the potential for carbon capture. The carbon dioxide byproduct of water-gas shift reactions exists in the same controlled environment as the hydrogen gas, meaning industrial facilities can trap the CO<sub>2</sub> before its release into the atmosphere. This approach manages to reduce pollution while supplying pure, energetic hydrogen, and catalysis research is essential to its success.



IBM's BlueGene/Q

#### Tools for Understanding Catalyst Structure and Function

One billionth of a meter can make the difference between a groundbreaking, highly efficient catalyst and one that fails to meet the needs of the growing energy economy. Fortunately, Brookhaven Lab researchers have access to collaborative facilities that probe those nanoscale characteristics and increase both the fundamental and applied understanding of these important catalysts.

The National Synchrotron Light Source not only reveals the nanoscale structure of materials, but its x-ray beamlines are capable of characterizing a catalyst in real time. Rather than analyzing just the initial and final states of a reaction, researchers can study in-situ precisely when the crucial phase of the reaction begins and how the catalyst performs throughout. When the National Synchrotron Light Source II begins operation in 2015, the x-ray intensity and analysis speed will climb considerably higher and allow the systematic study of catalysts under transient conditions.

The combined expertise of Brookhaven Lab's Chemistry Department and the Center for Functional Nanomaterials allows for the controlled synthesis of novel nanocatalysts and a detailed understanding of each element's role in a reaction.

As researchers seek more selective, efficient, and lower-cost chemical conversion techniques, custom-designed nanocatalysts offer new opportunities for performance breakthroughs. Advanced instruments such as transmission electron microscopes offer insight into catalyst structure, a critical component of advanced synthesis.

Over the past decade, growing computational power has transformed the practice of catalysis science. Calculations and simulations of atomic structure can now give reliable insight to map out chemical reactions and guide the design of better catalysts. In many ways, advanced computer modeling provides the key to the rational design of customized catalysts. Brookhaven's new supercomputer, IBM's cutting-edge BlueGene/Q, is one of the world's most powerful tools for aiding nanotechnology innovation.

With 600 teraflops of processing power, scientists are able to recreate the rapid reactions that happen during catalysis. Simulations illuminate the nanoscale arrangements and size-dependent structures behind the high-performance of the latest generation of energy catalysts.



SOLAR TO FUEL CONVERSION

Developing catalysts to mimic photosynthesis in the lab

While no single alternative energy source will completely meet the nation's energy needs, finding efficient ways to convert solar energy to fuels could be a large part of the solution.

Tapping into the sun in a variety of ways could help meet our nation's ever increasing energy needs. Engineering solar cells to convert sunlight into electricity and collecting solar heat are two common approaches. Brookhaven scientists are also working on another less well known but promising idea: converting solar energy to fuel by mimicking the way plants use sunlight energy to produce the molecules they need to live and grow. The goal of a man-made solar-to-fuels process is to produce useful liquid fuels directly using sunlight energy, and at higher overall efficiency than can be achieved at present by the conversion of plant matter to biofuels. We could then produce significant amounts of clean, renewable energy that would be usable where and when we need it, rather than only when the sun is out.

#### **Artificial Photosynthesis**

At first glance, natural photosynthesis sounds fairly simple: plants convert just three raw ingredients — energy from sunlight, carbon dioxide, and water — into carbohydrates and oxygen. Those carbohydrates fuel all the metabolic activities of the plants, the animals that eat the plants, and even our fossil-fuel burning cars and furnaces, which release the carbon stored in oil and coal via photosynthesis millions of years ago.

But there are many challenges to recreating this process in a laboratory. While plants use chlorophyll to absorb sunlight, scientists use metal complexes or semiconductors to absorb light and to separate electric charges. The separated charges initiate complex chemical reactions that store the solar energy as fuels such as hydrogen or carbon-based fuels such as methanol. Brookhaven chemists are working on

finding stable, visible-light absorbing chemicals and materials for use in photo-electrochemical cells.

#### Solar Water Splitting

One big challenge is finding efficient catalysts to drive the complex chemical processes needed to mimic photosynthesis in the laboratory. Catalysts must coordinate multiple electron, proton-, and atom-transfer processes to form new high-energy chemicals from thermodynamically stable precursors. This artificial photosynthesis challenge is linked to the broader chemistry challenge of using catalysts to activate stable, small molecules for chemical reactions.

One key process where an artificial photosynthesis catalyst is needed to produce a solar fuel is in "water splitting," or breaking water into

hydrogen and oxygen. The hydrogen atoms can then be used to form molecular hydrogen fuel. Water splitting requires a large amount of energy from sunlight, and effective metal catalysts to activate the very stable water molecules.

The overall water-splitting process occurs as two separate "half-reactions." In one, water oxidation produces molecular oxygen (O<sub>2</sub>), along with protons and electrons; in the other, the protons and electrons are combined to make molecular hydrogen (H<sub>2</sub>). These two half-reactions take place at different electrodes — the anode and the cathode — in a photo-electrochemical cell.

Brookhaven scientists, working with collaborators from the Institute for Molecular Science in Japan, have



Scientists synthesize and test new catalysts that can efficiently convert water into clean-burning hydrogen fuel.



Cutting-edge transmission electron microscopes probe the nanoscale structure of materials, opening new pathways for superior energy catalysts.

found a novel catalyst that appears promising for water oxidation: a ruthenium complex with bound quinone molecules. This compound efficiently catalyzes water oxidation to form oxygen through a very unique pathway in which the bound quinone molecules are actively involved. Also, in collaboration with researchers at the University of Houston, Brookhaven scientists recently discovered a low-energy pathway for the formation O<sub>2</sub>.

Another catalyst is needed for producing molecular hydrogen. Currently, platinum is the metal of choice as the catalyst for hydrogen production, but platinum is very expensive. Some bacteria employ hydrogenase enzymes to catalyze the production of hydrogen from water. These very efficient enzymes contain

the earth-abundant metals iron and nickel in their active sites. Brookhaven scientists, inspired by the hydrogenase examples, are exploring the use of less expensive and more abundant alternatives, including cobalt, nickel, and molybdenum.

#### **Carbon Dioxide Reduction**

Brookhaven researchers are also exploring the complicated catalytic processes of photosynthesis to see if they can find ways to transform carbon dioxide to fuels.

In the final stage of photosynthesis, plants convert carbon dioxide in the atmosphere into carbon-rich carbohydrates. A close collaboration of experimentalists and theorists from Brookhaven Lab and the Institute for Molecular Science (and now Kyoto

University) in Japan has been trying to mimic that process, but with carbonbased methanol as the end product.

The researchers submerged a lightabsorbing ruthenium catalyst that mimics an important substance in photosynthesis in an aqueous solution containing an electron donor. When irradiated with visible light, the catalyst produces a renewable hydride donor that can transfer a negative ion of hydrogen to a hydride-acceptor molecule.

The researchers found that the catalyst was able to pool the energy from two photons of light in the hydride donor. This catalyst is able to store two electrons generated by light and a proton as the hydride donor, which it can then transfer to an appropriate acceptor molecule. This process opens

the door to light-induced, catalytic hydride-transfer reactions for transforming carbon dioxide to methanol.

#### Liquid Hydrogen Storage

Another very promising route to a carbon-based fuel is to first produce  $\rm H_2$  by a solar driven process and then use a metal complex catalyst to reversibly convert the  $\rm H_2$  and  $\rm CO_2$  into an aqueous solution. This solution can be used to run a formic acid fuel cell, or as an efficient, liquid hydrogen-storage medium that can be transported for use in hydrogen fuel cells using the same kind of infrastructure used to transport other liquid fuels.

Brookhaven scientists recently developed an efficient non-precious-metal-based hydrogen evolution catalyst for the first step. Their formulation of nanosheets made of nickel, molybdenum, and nitrogen on a carbon electrode support results in a high surface area for chemical reactions, improved electronic properties of the nickel and molybdenum metals, and corrosion resistance even in strongly acidic solutions. A collaboration of scientists from Brookhaven and the National Institute of Advanced Industrial Science and Technology in Japan has also developed a metal complex catalyst with a proton-responsive ligand for

the second step for hydrogen storage. This catalyst works under very mild conditions, and can run the reaction converting  $\rm H_2$  and  $\rm CO_2$  into an aqueous solution in both forward or reverse directions — to store or release hydrogen — simply by changing the acidity of the solution.

There are still several hurdles on the path to solar-generated fuels, but Brookhaven's chemists are working on each challenge as it comes. If they can find catalysts that are both efficient and inexpensive, they may bring the world a big step closer to tapping the sun's energy.





# IMPROVING BIOFUEL PRODUCTION

Harnessing the power of plants and algae, nature's green factories

With expertise in plant biology, chemistry, computational modeling, environmental interactions, and biofuel conversions, Brookhaven scientists are exploring new ways to engineer plants to efficiently store and release energy.

When it comes to capturing and storing energy, plants are a natural. They use sunlight to convert carbon dioxide and water into carbohydrates and other products that fuel life on Earth. When we burn fossil fuels, we tap into a convenient source of energy locked up long ago by the plants and animals that decayed to form the rich and complex mixture of organic compounds comprising those fuels. But using fossil fuels for their energy content is not sustainable because they will eventually run out and there are environmental consequences. Also, burning this finite supply of precious organic compounds solely as a convenient source of energy permanently depletes a unique feedstock from which the materials (fibers and polymers), pharmaceuticals, and other products used in our daily lives are made. So forward-thinking scientists are looking for ways to engineer plants to efficiently store energy for more immediate use.

One key strategy is the exploration of biofuels — fuels produced directly by plants or derived from plant materials such as stalks, stems, seeds, and fruits. To improve biofuel production, scientists must learn how plants accumulate biomass and other products, and how to influence and optimize these processes. With expertise in plant genetics, metabolism, molecular biology, chemistry, computational modeling, and environmental interactions, scientists at Brookhaven Lab are making important contributions.

## Alternative Plants for Alternative Energy

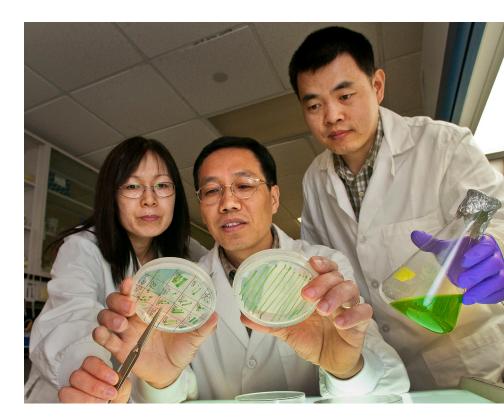
Ethanol, a form of alcohol produced by fermenting plant starches (e.g., corn), can be used as a direct replacement for gasoline. But corn-based ethanol diverts an important food source — and the

land it's grown on — to fuel production. A better approach would be to use non-food crops grown on non-agricultural land as the source for biofuels.

Brookhaven researchers are actively investigating several plant species, including grasses, aquatic plants such as duckweed, and fast-growing poplar trees, which have adapted to many different climates and habitats, including soil unfit for agricultural crops. They are also looking for ways to improve bioenergy crops' growth potential, particularly in less-than-ideal conditions.

Building on accomplishments in radiochemistry and imaging instrumentation in Brookhaven's unique integrated Plant Radiotracer Laboratory, researchers are exploring ways to improve plants' ability to thrive on marginal lands with increased resistance to drought, pests, and other environmental challenges. These studies use short-lived radioactive isotopes and non-invasive positron emission tomography (PET) imaging to monitor the movement of resources (including sugars and amino acids) — as well as key signaling hormones — to investigate the integrated functions of leaves, stems, and roots within intact growing plants.

The team has also developed a comprehensive portfolio of radiometric bioassays giving new insight into how and when plants use carbon and nitrogen resources. This combination of tools is allowing scientists to explore how plants' basic physiological and metabolic functions correlate with changes in gene expression and with changes in growth patterns to identify factors



Brookhaven researchers study cultures of algae that were shown to increase oil production in response to excess carbon.



that can improve plant hardiness, biomass accumulation, and carbon dioxide fixation.

#### **Breaking Down Walls**

Another key target of Brookhaven's research is to find ways to alter the composition of plant cell walls, the structural supports surrounding every plant cell. Plant cell walls can be broken down by enzymes into sugars that are suitable for fermentation into ethanol and other biofuels. But cell wall polymers are much more difficult to "digest" than starch, with some polymers (lignin) being harder to digest than others (cellulose, hemicellulose). So scientists are exploring ways to affect which polymers are made, and identifying new enzymes to modify cell wall structure for efficient breakdown.

Sophisticated imaging technologies are helping them explore the factors that partition plant nutrients between production of lignin, hemicellulose, and

cellulose. The goal is to tilt the balance away from extremely recalcitrant lignin toward hemicellulose and cellulose without compromising the plants' structural integrity. Analysis of the enzymes involved in the production of cell wall materials, including structural studies at Brookhaven's National Synchrotron Light Source (NSLS), have helped identify molecular targets and genetic engineering mechanisms for achieving this goal.

#### Oiling the Transition

Brookhaven researchers are also working on ways to increase the production of plant oils, which have more than twice the energy density of starch and could be used as feedstocks for the manufacture of alternative liquid fuels, such as biodiesel. Recent studies have uncovered how particular metabolites in the oil-making process work as signals to slow down production. The Brookhaven team is now looking for ways to interfere with this feedback

mechanism as one approach to get plants to make more oil.

The team is also working with collaborators to convert plants such as sugar cane into oil producers, using genetic techniques such as cross breeding with grasses to increase plants' productivity and potential for growing in nontropical regions. They've also found a way to coax photosynthetic green algae into pumping out more oil simply by feeding the microbes more carbon. This research overcomes a preconceived notion that algae growth and oil production were mutually exclusive, and could lead to the development of commercial strains of algae that generate biofuels more efficiently.

Tinkering with enzymes and metabolic pathways can also be used to modify plant oils for the direct production of biofuels, or to alter the fatty acid composition of existing biofuels. Since fatty acid composition affects many of the properties of biofuels — things like melting point and viscosity — the ability to strategically alter compositions could lead to improved properties.

In addition, Brookhaven scientists are using computational analysis to model the routes taken by carbon through plant metabolic networks so they can more accurately identify genetic and biochemical targets that can be modified to improve oil production.

#### Integrated Approach

This multidisciplinary exploration draws on strengths across scientific disciplines at Brookhaven Lab and emphasizes the flexibility inherent in a national laboratory setting for maximizing the impact of such integrated research. Collaborative projects with other DOE labs, universities across the nation, and nearby institutions such as Cold Spring



PET scans reveal the way plants store and move energy, helping scientists engineer better crops for use in renewable biofuels.



Embryos of the rapeseed plant accumulate seed oils — the most energy-dense form of biologically stored sunlight — which have great potential as renewable resources for fuel and industrial chemicals.

Harbor Laboratory and Stony Brook University will build on these results.

The effort to identify and tailor make new energy sources from plants and algae could make valuable contributions to our nation's future energy needs. But biofuel science will not solve the energy challenge in a vacuum. Like all new technologies, bioenergy will have to be developed in a sustainable way, with consideration given to how science intersects with a wide range of factors, including economic and cultural interests — the aforementioned balance between food and fuel production, land and water use, potential effects on biodiversity, geographic variability, and infrastructure needs, to name a few.

Achieving a positive carbon balance illustrates the complexity of these issues: Using plants as a resource for carbon-based fuels could result in an improved carbon "budget" for our planet because the carbon released by burning biofuels was only recently removed from the atmosphere — as compared to that stored millennia ago in fossil fuels. But if the crops used to generate biofuels require energy-intensive agriculture and diversion of

other essential resources, some of the benefits of bioenergy could be offset by these unintended consequences.

It will therefore be important to incorporate understanding of these complex, interconnected issues as we strive to apply what we learn from science toward achieving a greener planet.

### Thermochemical Conversion of Plants into Power

Biomass — organic matter most often made from trees and other plants provides an abundant source of renewable energy. Often, biomass is directly incinerated and its intrinsic energy is released as heat, as in the case of campfires and wood-burning stoves. But industrial processes can convert biomass into liquid or gaseous biofuels, which can then be upgraded and substituted for petroleum-based alternatives. Critically, this energy source is currently the only one that can be integrated into existing carbon-based energy systems as a sustainable alternative, although scientists are also working on direct solar-to-fuels processes.

Brookhaven Lab leads the exploration and optimization of biomass thermal

conversion processes for plants native to the Northeast, strengthening the potential positive impact on the regional economy. Researchers take samples provided by the State University of New York at Syracuse — including maple, poplar, and switch grass — and convert them into biofuels. The Lab is pursuing the development of two thermochemical conversion processes: one, called pyrolysis, rapidly heats the samples to around 500 degrees Celsius, converting 70 percent of the material into condensable liquid fuel; the other, called gasification, heats the biomass to 900 degrees Celsius and produces a synthesis gas of carbon monoxide, hydrogen, and light hydrocarbons such as methane.

In the Brookhaven bench-scale research projects, microgram samples of biomass are subjected to thermochemical conversion while being measured by a customized gas chromatograph and mass spectrometer, which analyzes their precise composition and helps determine their ultimate energy potential. Improvements to the chemical process then hinge upon the development of customized catalysts for both pyrolysis and gasification.



BROOKHAVEN LAB'S FACILITIES AND SOLUTION CENTERS

Building and operating today's tools for tomorrow's discoveries

Brookhaven National Laboratory is known for the design, construction, and operation of large-scale, cutting-edge research facilities used by scientists from around the world.

Each year, thousands of scientists from laboratories, universities, and industries across the U.S. and around the world come to Brookhaven to use our cuttingedge research facilities. These tools some available nowhere else on the planet — allow them to delve into the basic mysteries of physics, chemistry, biology, materials science, energy, and the environment — and develop innovative applications that arise at the intersections of these disciplines. The facilities highlighted below are already playing a prominent role in the quest for solutions to key energy challenges.

Center for Functional **N**anomaterials

Brookhaven's Center for Functional Nanomaterials (CFN) provides state-ofthe-art capabilities for the fabrication and study of nanoscale materials, with an emphasis on atomic-level tailoring to achieve desired properties and functions. Nanoscience has enormous promise in developing solutions to our energy challenges because the processes of energy production, conversion, and use — from the movement of electrons to the catalysis of reactions that convert energy from one form to another — all occur at the nanoscale. Basic research aimed at understanding the details of these processes and structures will enable scientists to design and engineer improvements to optimize efficiency and performance across the spectrum of energy production, transmission, storage, and use.

#### **National Synchrotron** Light Source and NSLS-II

One of the world's most widely used scientific research facilities, the National Synchrotron Light Source (NSLS) provides intense beams of light to gain information about the electronic and atomic structures of materials, analyze very small samples, or study surfaces at

the atomic level. NSLS will be replaced in 2015 by the next-generation NSLS-II, which will be 10,000 times brighter than the existing NSLS, allowing studies of even greater precision. The advanced capabilities of NSLS-II will allow scientists to see materials at

the scale of a nanometer — a billionth of a meter — a capability not available at any other light source in the world. Working at the nanoscale, researchers will focus on some of the nation's most important scientific challenges in developing clean, affordable energy.



Center for Functional Nanomaterials



National Synchrotron Light Source II

#### Interdisciplinary Science Building

This state-of-the-art facility, completed in 2013, is a new hub for energy research at the Laboratory, providing customized laboratories for crossdisciplinary teams of scientists working to engineer and optimize materials for new battery, biofuel, and photovoltaic technologies. The building contains 60 standard laboratories and four specialty labs with unique features, including a dry room with finite humidity control, where researchers can assemble and test new lithium-ion batteries; two ultralow vibration laboratories housing a scanning tunneling microscope used to explore materials' electronic structure at the atomic scale; and a lab customized for molecular beam epitaxy (MBE) a process researchers use to fabricate new materials a single atomic layer at a time — connected directly to one of the ultra-low vibration labs via a vacuum-locked system. This allows

scientists to transport MBE-created samples directly to the microscope without exposing them to air, which can diminish sought-after properties.

#### The Smarter Grid Research, Innovation, Development, Demonstration, Deployment Center (SGRID<sup>3</sup>) and AEGIS

In an effort to design and implement our next-generation power grid, Brookhaven Lab and Stony Brook University are developing a joint center that will function as a grid laboratory to support new grid technologies and their commercialization. Challenges include integrating a growing number of renewable energy resources into the grid, providing for increased electrification of vehicles, and the need for better transmission and storage systems grid-wide. SGRID<sup>3</sup> aims to accelerate breakthrough technologies in smart grid devices and the future construction, operation, and control of electric

power transmission and distribution systems. The center will also create an infrastructure for development and testing of new technologies, equipment, and components to guide future utility investments in New York State.

At Brookhaven, the primary SGRID<sup>3</sup> facility will be the planned Advanced Electrical Grid Innovation and Support Center (AEGIS), which will facilitate development of new capabilities to allow utilities to monitor and model their grids in real time — a capability that currently does not exist. AEGIS will enable researchers and utility representatives to develop knowledge that will guide future utility investments in the electrical transmission and distribution systems in the Northeast, and will also provide advanced computing capabilities for grid studies and simulations focused on natural and unnatural events.



Interdisciplinary Science Building



#### Long Island Solar Farm (LISF)

The Long Island Solar Farm is a 32-megawatt solar photovoltaic power plant built through a collaboration including BP Solar, MetLife, the Long Island Power Authority (LIPA), and the Department of Energy. The LISF, located on the Brookhaven Lab site, began delivering power to the LIPA grid in November 2011, and is currently the largest solar photovoltaic power plant in

the Eastern United States. It is generating enough renewable energy to power approximately 4,500 homes, helping New York State meet its clean-energy and carbon-reduction goals. Data from this facility give Lab scientists a unique opportunity to study solar variability and impact, grid integration, and the potential environmental impacts of such solar arrays.

#### Northeast Solar Energy Research Center

The Northeast Solar Energy Research Center (NSERC) will be a solar photovoltaic research array where researchers from Brookhaven and other national labs, academia, and industry will test new technologies for collecting solar energy and making it available for use as efficiently and economically as possible. The test array will enable realworld, utility-scale tests of advanced "smart grid" ready technologies to foster increased amounts and better

integration of solar power on utility distribution systems. The NSERC array will produce between 700 kilowatts (kW) and one megawatt (MW) of electric power that will be used at Brookhaven, but its real value will be the research it enables to help improve solar efficiency, particularly in the Northeast.

#### **Brookhaven Microgrid**

NSERC will be a key part of the Brookhaven microgrid, which will use a portion of the Lab's campus and electrical infrastructure as a test bed for smart grid technologies, such as smart grid sensors. This on-site microgrid will be used by researchers, utilities, and industry as a test bed for new transmission, storage, sensing, and integration technologies.

By observing how the Lab's grid works, researchers will be able to get performance data, analyze it, and bring together advanced modeling capabilities to learn how to save power and improve efficiency.

#### Solution Centers

#### Matching research needs with facilities, capabilities and expertise

Brookhaven is establishing a series of "Energy Solution Centers" that would take advantage of its unique scientific capabilities and expertise to take on key energy research issues identified by academia and industry.

The Centers will integrate the broad suite of capabilities and expertise available at NSLS, NSLS-II, CFN, and NSERC to address these key research challenges. This is of particular importance, for example, in the nanoscale world, where data from a single experiment often does not provide sufficient information to answer a scientific question. By combining information from complementary instruments, however,

The Lab's Energy Solution Centers will integrate the broad suite of capabilities and expertise available at Brookhaven Lab facilities, including the CFN, to take on key energy research issues identified by academia and industry.

these Centers can provide a much more complete understanding of the relationship between structure and function in nanomaterials, leading to advances that may not have been possible elsewhere.

The Centers will feature capabilities primarily targeted at the materials science and chemical science research communities. They'll also create an environment of greater communication and interaction among Brookhaven facility and core-program researchers and key academic/industrial scientists. This will allow a stronger link between the scientific "seeds" produced by the discovery-focused scientists at the Lab and the technological needs of the deployment-focused researchers in industry.

One example of the Solution Center philosophy in action is Brookhaven and Stony Brook University's battery and storage initiative. Led by a joint Stony Brook/Brookhaven appointee, the effort will focus on extending grid- and vehicle-scale battery lifetimes through the exploration of new battery chemistries. An integrated team of academic and industrial scientific leaders and world-class materials science experts will work together to leverage DOE's investments in state-of-the-art photon science and nanoscience facilities at Brookhaven (NSLS, NSLS-II, and CFN). The collaborations will accelerate the translation of experimental knowledge into commercial products.

Brookhaven's Solution Centers would build on recent DOE and Brookhaven-led workshops with representatives of energy research communities focused on issues relevant to DOE's energy mission in the areas of catalysis, photovoltaics, and advanced materials for energy storage and distribution. These workshops produced a matrix for each research area identifying that community's scientific issues and mapping them to the Laboratory's facility capabilities and expertise. Brookhaven is focusing its facility investments to meet these community needs, enabling greater scientific impact through engagement.

#### **ENERGY INNOVATION at Brookhaven National Laboratory**

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One of ten national laboratories overseen and primarily funded by the Office of Science of the U.S. Department of Energy (DOE), Brookhaven National Laboratory conducts research in the physical, biomedical, and environmental sciences, as well as in energy technologies and national security. Brookhaven Lab also builds and operates major scientific facilities available to university, industry and government researchers. Brookhaven is operated and managed for DOE's Office of Science by Brookhaven Science Associates, a limited-liability company founded by the Research Foundation for the State University of New York on behalf of Stony Brook University, the largest academic user of Laboratory facilities, and Battelle, a nonprofit applied science and technology organization.



